

ELECTROSTATIC DISPERSION AND EVAPORATION OF DENSE AND DILUTE CLUSTERS OF DROPS OF HIGH-ENERGY FUEL FOR SOOT CONTROL¹

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INTRODUCTION

The high-energy-density (HED) fuels developed under U.S. Navy sponsorship as a replacement for conventional liquid fuels in its missile propulsion systems have the drawback of high soot propensity: this makes missiles visible and thus strategically unacceptable. Experimental evidence of heavy sooting from such potential fuels has been presented by Law[1]. Soot propensity is defined here as the ability of a fuel to form soot precursors through nucleation reactions; it does not refer to soot growth, or soot production which includes the additional effect of soot destruction through oxidation reactions.

The general goal of this study is to investigate the potential for reducing soot propensity through the reduction in soot nucleation reactions which are the initiators of soot formation processes. The concept employed is electrostatic liquid drop charging for dispersing drops so as to avoid the creation of the fuel-rich-vapor regions where soot nucleation occurs. The relation between drop dispersion and soot formation has been experimentally investigated by Sangiovanni and Liscinsky [2] who showed that the soot emission index decreases monotonically with the spacing between drops in a stream. The results were consistent for a variety of fuels and oxygen mass fractions in the surrounding gas. Since in that study [2] it is only the effect of drop spacing in a single direction that has been investigated, those results underestimate the benefit of drop dispersion in a real spray where a drop is surrounded by other drops in all directions.

The previous two years studies have focussed on: (1) calculations of fuel properties [3], (2) proof of the concept [4], and (3) elucidation of velocity effects (is it soot propensity reduction, or could it be soot oxidation effects) [5]. This year has been focussed on: (1) calculation of additional fuel properties (more recent fuels used by Law [6]), and (2) binary fuel effects where only one of the fuels is a HED fuel.

MODEL

The model is based upon the cluster-in-vortex model of Harstad and Bellan [7] and the model of solvent/solute evaporation of Harstad and Bellan [8]. Since it is the binary fuel aspect that is of interest here, it is this model that is briefly described below.

The two main assumptions of the model is that the solute is much more volatile than the solvent (once at the drop surface, the solute evaporates immediately) and that the mass fraction of solute is smaller by almost an order of magnitude than that of the solvent. In general, the evaporation rate is the sum of three terms: the evaporation rate of the solvent according to the Langmuir-Knudsen (L-K) evaporation law, the diffusion rate of the solute through the boundary layer and the rate of surface layer stripping of the solute. However, two important limiting regimes of evaporation are identified according to the value of a dimensionless number $Be \equiv -[R/(D_m u_l)]^{0.5} (dR/dt)$ that represents the ratio of the mass regression rate to a characteristic volatile diffusion rate; R is the drop radius, D_m is the liquid mass diffusivity, u_l is the velocity of the liquid inside the drop and t is the time. When $Be \ll 1$, diffusion into the boundary layer governs the rate of species transfer from the liquid core to the drop surface; subsequent mass transfer from the drop surface to the gas phase is governed by evaporation according to the L-K evaporation law. These are sequential processes and the overall mass transfer is determined by the lower of the diffusion and evaporation rates. In contrast, when $Be \gg 1$, transfer of the solute from the liquid core to the gas phase is governed by the rate of surface layer stripping (the evaporation rate of the drop). Because surface layer stripping and diffusion rate from the core to the boundary layer are competitive processes, the overall transfer of solute from the core to the gas is governed by the higher of the diffusion and drop regression rates. The quasi-steady boundary layer assumption is consistent with $Be \ll 1$ but inconsistent with $Be \gg 1$. Results from previous simulations show that dilute clusters of drops evaporate in the $Be \ll 1$ regime whereas dense clusters of drops evaporate mostly in the $Be \gg 1$ regime.

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SIMULATIONS RATIONALE

Early experiments with cubane by Law [1] pointed out one of the main drawbacks of cubane as a liquid propulsion fuel: in solution with other fuels it does not participate in combustion and instead it accumulates in the fuel cresting an increasingly viscous, less volatile mixture until supersaturation occurs when a temperature larger than the boiling point of the more volatile fuel is attained. It is only at that time that microexplosions ensue and cubane participates in the burning process. To palliate this aspect of cubane, liquid cubane compounds were synthesized and studied. For example, experiments by Law [6] at $p = 0.25$ atm showed that methylcubane (MTCU) has a considerably larger burning rate constant, K , than nonane (NONA), a typical hydrocarbon; experiments were also performed with pure nonane and pure MTCU showing the increase in K with p , and with mixtures of nonane/MTCU. The rationale of using mixtures of a HED fuel and a typical hydrocarbon is that HED fuels are expensive and thus might not be economically feasible to use; judiciously used in solution with a hydrocarbon they might still enhance burning, yet be more economical.

Taking guidance from the experiments of Law [6], MTCU was chosen as a typical HED to be used as a solute in a mixture with a hydrocarbon. Following the methods previously outlined [3], the properties of MTCU were estimated as seen in Table 1. Plots of the saturation pressure versus the temperature for benzvalene (BV), quadricyclane (QUAD), dihydrobenzvalene (DHBV), MTCU, heptane (HPT) and NONA appear in Fig. 1. These plots show that the difference in volatility between MTCU and NONA is such that at for Law's experimental conditions of $p = 0.13$ atm and 0.25 atm, MTCU is more volatile than NONA and thus the mixture NONA/MTCU is indeed a reasonable solvent/solute mixture. However, for $p > 1$ atm, it is NONA that is more volatile than MTCU and the entire concept of the HED being used as a solute breaks down. Moreover, it appears that for $p > 1$ atm MTCU is the least volatile of the substances considered here and thus it cannot serve as a solute in any combination with them.

Since the previous conclusion is a direct result of the estimated MTCU properties, a calculation was carried out with the cluster-in-vortex model exercised in the very dilute regime to attempt duplicating the pure MTCU results of Law [6] at $p = 0.13$ atm and 0.25 atm. This validation should be viewed with caution because the model of the cluster-in-vortex can break down in the very dilute regime as it was derived primarily for the dense regime. Calculations were performed with a cluster of uniformly-distributed, monodisperse drops of 0.438 μm diameter at 0.13 atm and of 0.531 μm diameter at 0.25 atm in a vortex embedded into a very hot T environment (3000 K) to duplicate the high flame temperature of MTCU (which however had not been

measured [6]). The cluster radius was 2 cm; both the vortex and the drops had negligible velocities [$0(10^{-3})$ cm] to duplicate the collection-free environment of the experiment. The calculations at 0.13 atm yielded $K = 1.125$ mm^2/s which should be compared to the experimental value of 1.2 mm^2/s . Calculations at the higher pressure (0.25 atm) could not be completed due to convergence problems as the model and code have not been derived for the very dilute regime. However, even the limited agreement at $p = 0.13$ atm is an indication that there is some validity to the calculated properties (Table 1 and Fig. 1).

Further examination of Fig. 1 showed that NONA is considerably less volatile than BV, QUAD or DHBV and thus was chosen to represent the solvent while the other three fuels were used as solutes. The results of the calculations were used to examine the evolution of the partial fuel density: (1) effect of the solute for uncharged drops, (2) effect of the solute for charged drops, and (3) fuel specific effects for charged drops; these results will be reported at the meeting.

References

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Symbol	BV	QUAD	DHBV	MTCU
$\Phi_s \equiv (\text{air/fuel})$ mass	13.2	13.4	13.7	13.4
w , g/mole	78.12	92.14	80.14	118
T_{bn} , K	353	382	344	423
L_{bn} , cal/g	96.90	96.85	74.50	58.1
ΔC_p , cal/(gK)	6.8×10^{-2}	1.48×10^{-3}	0(assm)	0(assm)
ρ_l , g/cm ³	0.879	0.7	0.71	0.908
C_{pl} , cal/(gK)	0.415	0.36	0.432	0.2
μ_l , g/(ems)	0.392×10^{-2}	0.316×10^{-2}	0.35×10^{-2} (assm)	0.35×10^{-2} (assm)
$D_{ml}(Le_l=10)$, cm ² /s	0.995×10^{-4}	0.999×10^{-4}	0.978×10^{-4}	1.27×10^{-4}
λ_l , cal/(gK)	3.63×10^{-4}	2.67×10^{-4}	3×10^{-4}	2.44×10^{-4}
$C_{pg}(T_g = 424 \text{ K})$	0.37	0.435	0.437	0.4

Table 1: Properties of high-energy fuels

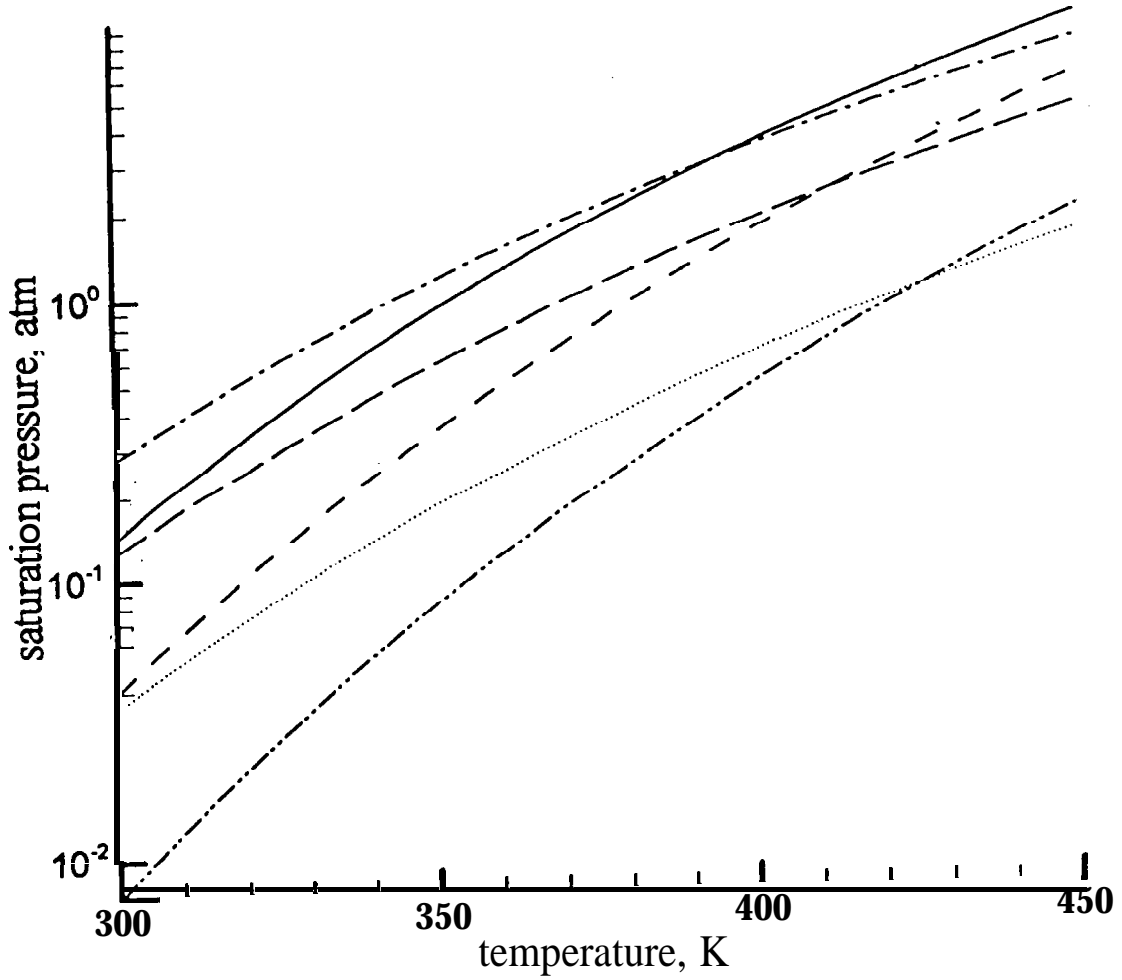


Figure 1. Saturation pressure versus temperature for BV(—); QUAD (- - -); DHBV (- . - .); MTCU (. . .); HPT (- - -); NONA (- . . -).